



chain nodes :

6 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 42 43  
48 49 52

ring nodes :

1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18

chain bonds :

2-42 3-6 4-52 6-43 7-23 7-31 8-24 8-30 9-20 9-29 11-21 11-32 12-22 12-33 13-27  
13-36 14-28 14-37 15-19 17-25 17-34 18-26 18-35 19-39 20-38 48-49

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17  
17-18

exact/norm bonds :

1-2 1-5 2-3 2-42 3-4 4-5 4-52 6-43 7-8 7-12 7-23 8-9 8-24 9-10 10-11 11-12  
11-21 12-22 13-14 13-18 13-27 14-15 14-28 15-16 16-17 17-18 17-25 48-49

exact bonds :

3-6 7-31 8-30 9-20 9-29 11-32 12-33 13-36 14-37 15-19 17-34 18-26 18-35 19-39  
20-38

G1:[\*1],[\*2]

G2

G3:N,Cy,Hy,[\*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS 21:CLASS  
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS  
31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS  
42:CLASS 43:Atom 48:CLASS 49:CLASS 52:CLASS